Ethofumesate 26225-79-6 | DTXSID8034580

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Model Performance

Model	Data
Widdel	Data

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.95	0.69	0.95	0.65	0.96	0.68	

Model Results

Predicted value: 7.79

Global applicability domain: Inside

Local applicability domain index: 9.46e-01

Confidence level: 8.39e-01

Nearest Neighbors from the Training Set

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4,4'-Dichlorobiphenyl Measured: 7.68 Predicted: 7.38

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2,2'-Dichlorobiphenyl Measured: 7.18 Predicted: 7.38

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2,4'-Dichlorobiphenyl Measured: 7.40 Predicted: 7.38

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1,2,3,4-Tetrachloronaphthalene

Measured: 8.30 Predicted: 8.41

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2,3-Dichlorodibenzo-4-dioxin

Measured: 8.50 Predicted: 8.49